DOCTORAL THESIS

# Bayesian surrogates for functional response modeling and metamaterial rapid design

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# Abstract

In many scientific and engineering researches, Bayesian surrogate models are utilized to handle nonlinear data for regression and classification tasks. In this thesis, we consider a real-life problem, functional response modeling of metamaterial and its rapid design, to which we establish and test such models. To familiarize with this subject, some fundamental electromagnetic physics are provided.

Noticing that the dispersive data are usually in rational form, a two-stage modeling approach is proposed, where in the first stage, a universal link function is formulated to rationally approximate the data with a few discrete parameters, namely poles and residues. Then they are used to synthesize equivalent circuits, and surrogate models are applied to circuit elements in the second stage.

To start with a regression scheme, the classical Gaussian process (GP) is introduced, which proceeds by parameterizing a covariance function of any continuous inputs, and infers hyperparameters given the training data. Two metamaterial prototypes are illustrated to demonstrate the methodology of model building, whose results are shown to prove the efficiency and precision of probabilistic predictions. One well-known problem with metamaterial functionality is its great variability in resonance identities, which shows discrepancy in approximation orders required to fit the data with rational functions. In order to give accurate prediction, both approximation order and the presenting circuit elements should be inferred, by classification and regression, respectively. An augmented Bayesian surrogate model, which integrates GP multiclass classification, Bayesian treed GP regression, is formulated to provide a systematic dealing to such unique physical phenomenon. Meanwhile, the nonstationarity and computational complexity are well scaled with such model.

Finally, as one of the most advantageous property of Bayesian perspective, probabilistic assessment to underlying uncertainties is also discussed and demonstrated with detailed formulation and examples.

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